

## **ABSTRACT**

**THESIS:** Testing the Tran-Blaha Approach for Band Gap Calculations in a Pseudo-potential Environment

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**DATE:** December 2015

**PAGES:** 88

This study investigates the performance of the Tran-Blaha (TB) method for pseudo-potential calculations of semiconductor and metallic systems, using conventional Density Functional Theory (DFT) approximations to model interactions. DFT is a widely used tool that makes accurate ground-state energy calculations of electronic systems. It yields precise predictions of lattice constants, bulk moduli, and cohesive energies. However, one problem of conventional DFT is that it significantly underestimates band gap energies, hence the desire to test a new method, the TB method. This work is achieved with a database of pseudo-potentials that accurately reproduces all-electron calculations of ground state properties, and the plane-wave pseudo-potential code, ABINIT. The TB method is then used as a correction to valence orbital energies. This enables one to determine band structure, band gap energies, and density of states. Additionally, the effect of this model on the energy of d-state bands is analyzed, since the TB method struggles to accurately represent these bands, as well as the dependence of band gap values on lattice constants.